

beta-Caryophyllene

87-44-5 | DTXSID8024739

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 6.90

Global applicability domain: Inside

Local applicability domain index: 9.64e-01

Confidence level: 7.31e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,2-Dichloronaphthalene</div> <div>Measured: 6.89</div> <div>Predicted: 6.90</div>	<div>Image not found</div> <div>trans-Stilbene</div> <div>Measured: 7.48</div> <div>Predicted: 6.90</div>	<div>Image not found</div> <div>1,5-Dichloronaphthalene</div> <div>Measured: 6.65</div> <div>Predicted: 6.90</div>
<div>Image not found</div> <div>1,4-Dichloronaphthalene</div> <div>Measured: 6.78</div> <div>Predicted: 6.90</div>	<div>Image not found</div> <div>2,7-Dichloronaphthalene</div> <div>Measured: 6.70</div> <div>Predicted: 6.90</div>	